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POLARIZATION SENSITIVE CARS SPECTROSCOPY AND CONFORMATIONAL ANALYSIS OF ORGANIC MOLECULES IN LIQUIDS*

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ABSTRACT.

The paper presents the results of experimental investigations of a series of conformationally inhomogeneous compounds with polarization sensitive coherent active (anti-Stokes) Raman scattering spectroscopy (PS CARS). Interpretation of vibrational spectra are refined and spectroscopic parameters are determined of resonances of complex spectral band of n-penthane (bands at 868 and 841 cm^{-1}), 5,5-dimethil, 2-ethinyle, 1,2-dioxane (bands at 949 and 910 cm^{-1}) which were not resolved previously with use of spontaneous Raman scattering spectroscopy (SRS). On the basis of the conformational analysis of thio- and selenanisole by the PS CARS method, it was concluded that molecules involved exist predominantly in one isomeric form. Thereby the principle of holographic spectroscopic was realized and tested in the full scale.

INTRODUCTION.

Existence of complex molecules in several conformational states with different spatial positions of structural subunits results in production of extra lines in vibrational spectra, i.e. new lines which are not predicted by the group analysis of vibrations of molecule with fixed structures. However, the frequencies of normal vibrations of different conformations differ very slightly and are not resolved in ordinary spectra. Hence, the vibrational spectra without extra lines may be explained by the presence of several conformations with practically identical spectra. This fact restricts the potentialities of vibrational spectroscopy –IR absorption and spontaneous Raman scattering (SRS) – in conformational analysis.

As it will be demonstrated later, the sensitivity and the amount of information obtained in the conformational analysis of vibrational spectra may be essentially improved if using the

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* Dedicated to Professor Paraskeva Simova